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=> file casreact
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FILE CONTENT:1840 - 27 Oct 2007 VOL 147 ISS 19

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*                                                          *
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*                                                          *
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database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d que
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L2          133 SEA FILE=CASREACT SSS FUL L1 (   568 REACTIONS)
L3            4 SEA FILE=CASREACT L2 AND (ZIRCONIU? OR HAFIU?)


=> d l3 1-4 ibib abs fcrd


L3   ANSWER 1 OF 4  CASREACT  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         147:257772  CASREACT
TITLE:                    Process for preparation of chiral benzimidazolyl
                          pyridylmethyl sulfoxides from the corresponding
                          sulfides using chiral transition metal complexes and
                          oxidizing agents.
INVENTOR(S):              Dubey, Sushil Kumar; Vig, Gaurav; Singh, Anand;
                          Tripathi, Sushil; Paul, Soumendu
PATENT ASSIGNEE(S):       Jubilant Organosys Limited, India
SOURCE:                   PCT Int. Appl., 21pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2007088559      A1   20070809       WO 2007-IN35     20070131
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
             KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
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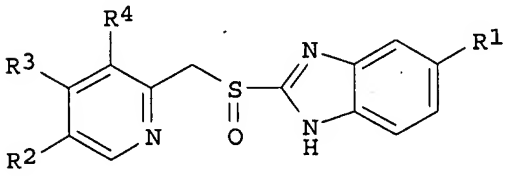
MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM

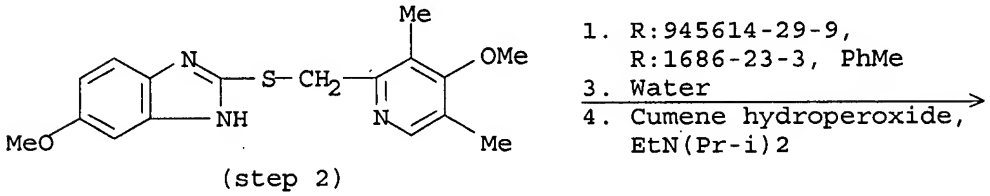
PRIORITY APPLN. INFO.: IN 2006-DE271 20060201
OTHER SOURCE(S): MARPAT 147:257772
GI



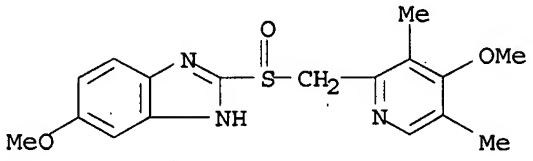
I

AB Title compds. (I; R1-R4 = H, alkyl, alkoxy, aryl, aryloxy), were prepared by treatment of the corresponding prochiral sulfides with chiral transition metal complexes and oxidizing agents optionally in presence of an organic solvent, wherein the chiral ligands comprise dicyclohexylidene, diacetonide, or benzylidene derivs. of sugars. Thus, vanadium oxytripropoxide and 1,2,4,5-Di-O-cyclohexylidene-D-fructofuranose were stirred together for 10-15 min in PhMe; 5-methoxy-2-[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]thio]-1H-benzimidazole and H2O were added and the mixture was heated at 50-55° for 1 h; the mixture was cooled to 25-30° followed by addition of diisopropylethylamine and cumene hydroperoxide over 1 h followed by stirring for 45 min. and workup to give 5-methoxy-2-[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole, sodium salt in 75% enantiomeric excess.

RX(1) OF 1



(step 2)



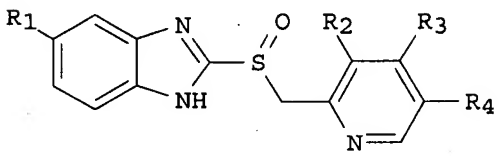
NOTE: alternative preparation shown, stereoselective
CON: STAGE(1) 10 - 15 minutes, room temperature
STAGE(2) room temperature -> 55 deg C
STAGE(3) 1 hour, 50 - 55 deg C; 55 deg C -> 30 deg C
STAGE(4) 1 hour, 25 - 30 deg C; 45 minutes, 25 - 30 deg C

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

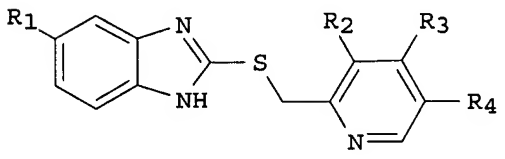
L3 ANSWER 2 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 144:390922 CASREACT
TITLE: Stereoselective oxidation processes for the preparation of chiral substituted sulfoxides from the racemic sulfides
INVENTOR(S): Kumar, Neela Praveen; Khanna, Mahavir Singh; Prasad, Mohan; Kumar, Yatendra
PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006040635	A1	20060420	WO 2005-IB2946	20051004
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1802584	A1	20070704	EP 2005-790107	20051004
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
IN 2007DN03340	A	20070831	IN 2007-DN3340	20070503
PRIORITY APPLN. INFO.:			IN 2004-DE1957	20041011
			WO 2005-IB2946	20051004

OTHER SOURCE(S): MARPAT 144:390922
GI



I

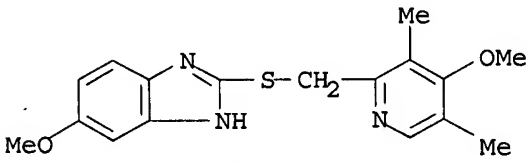


II

AB An enantioselective catalytic oxidation process for the preparation of an optically active enantiomer or an enantiomerically enriched form of a substituted pyridinylmethylsulfinylbenzimidazole [I; R1-R4 = H, C1-4 (un)branched alkyl, C1-4 (un)branched alkoxy, aryl, aryloxy], or its pharmaceutically acceptable salts (e.g., esomeprazole potassium), comprises oxidizing a prochiral sulfide (II; e.g., omeprazole sulfide) in

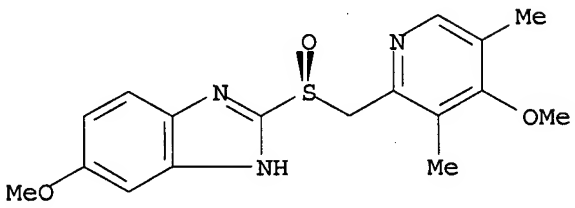
the presence of a chiral transition metal complex [e.g., titanium isopropoxide and L-(+)-diethyl tartrate] and a base (e.g., diisopropylethylamine) in the absence of an organic solvent with an oxidant (e.g., cumene hydroperoxide) followed by an optional salification (e.g., potassium hydroxide).

RX(1) OF 3



(step 2)

1. Ti(OPr-i)4, Di-Et L-tartrate
2. Cumene hydroperoxide, Di-Et L-tartrate, EtN(Pr-i)2
3. KOH, MeOH



K

NOTE: optimization study, stereoselective
CON: STAGE(1) room temperature -> 50 deg C; 1.5 hours; 25 - 30 deg C
STAGE(2) 25 - 30 deg C; 3 hours, 25 - 30 deg C
STAGE(3) 25 - 35 deg C; 15 - 16 hours, 25 - 35 deg C

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 144:51582 CASREACT
TITLE: Process for the preparation of pyridin-2-ylmethylsulfinyl-1H-benzimidazoles via oxidation of the corresponding sulfides in the presence of zirconium or hafnium complexes.
INVENTOR(S): Kohl, Bernhard; Mueller, Bernd; Weingart, Ralf Steffen
PATENT ASSIGNEE(S): Altana Pharma AG, Germany
SOURCE: PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005118569	A1	20051215	WO 2005-EP52471	20050531

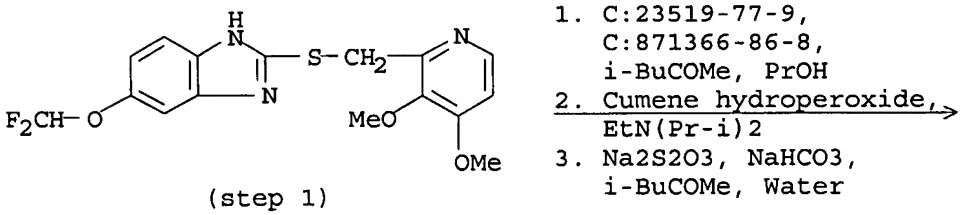
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

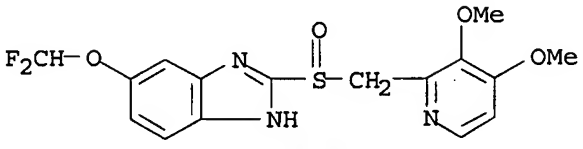
AU 2005250175	A1	20051215	AU 2005-250175	20050531
CA 2568652	A1	20051215	CA 2005-2568652	20050531
EP 1758889	A1	20070307	EP 2005-752651	20050531
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
CN 1960987	A	20070509	CN 2005-80017526	20050531
US 2007225500	A1	20070927	US 2006-597373	20061122
KR 2007031945	A	20070320	KR 2006-726831	20061220
IN 2006MN01589	A	20070615	IN 2006-MN1589	20061220
NO 2006006003	A	20061222	NO 2006-6003	20061222
PRIORITY APPLN. INFO.:			EP 2004-102467	20040602
			WO 2005-EP52471	20050531

AB A process for preparing mixts. of enantiomers of proton pump inhibitors (PPIs) having a sulfinyl structure comprises oxidation of the corresponding sulfides in the presence of a mixture of enantiomers of chiral zirconium or hafnium complexes. Thus, 5-difluoromethoxy-2-[(3,4-dimethoxy-2-pyridinyl)methylthio]-1H-benzimidazole was heated with DL-tartaric acid bis(N-pyrrolidinamide) and zirconium tetra-n-propoxide in Me iso-Bu ketone at 40° for 1 h followed by addition of diisopropylethylamine and slow addition of cumene hydroperoxide to give 75% 5-difluoromethoxy-2-[(3,4-dimethoxy-2-pyridinyl)methylsulfinyl]-1H-benzimidazole.

RX(1) OF 1



(step 1)



75%

NOTE: optimization study
CON: STAGE(1) 1 hour, 40 deg C; 40 deg C -> room temperature
STAGE(2) room temperature; 5 - 24 hours, room temperature

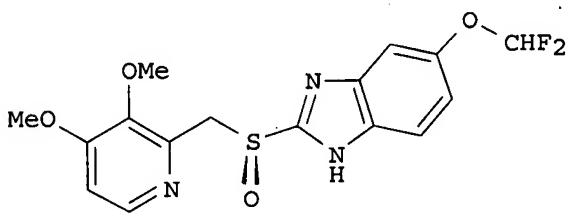
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:54346 CASREACT
TITLE: A process for preparing (S)-pantoprazole via stereoselective oxidation of pyridinylmethylsulfinylbenzimidazole derivative in the presence of L-tartaric acid derivative and chiral zirconium or hafnium catalyst

INVENTOR(S): Kohl, Bernhard; Mueller, Bernd; Weingart, Ralf Steffen
PATENT ASSIGNEE(S): Altana Pharma Ag, Germany
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004052881	A2	20040624	WO 2003-EP13604	20031203
WO 2004052881	A3	20041104		
W: AE, AL, AU, BA, BR, CA, CN, CO, DZ, EC, EG, GE, HR, ID, IL, IN, IS, JP, KR, LT, LV, MA, MK, MX, NO, NZ, PH, PL, SG, TN, UA, US, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2507889	A1	20040624	CA 2003-2507889	20031203
AU 2003293749	A1	20040630	AU 2003-293749	20031203
EP 1575941	A2	20050921	EP 2003-789113	20031203
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003016702	A	20051018	BR 2003-16702	20031203
CN 1717402	A	20060104	CN 2003-80104409	20031203
JP 2006514985	T	20060518	JP 2005-502309	20031203
MX 2005PA05761	A	20050816	MX 2005-PA5761	20050530
IN 2005MN00673	A	20051021	IN 2005-MN673	20050627
US 2006167262	A1	20060727	US 2005-536891	20051125
PRIORITY APPLN. INFO.:			EP 2002-27274	20021206
			DE 2003-10340254	20030829
			WO 2003-EP13604	20031203

GI



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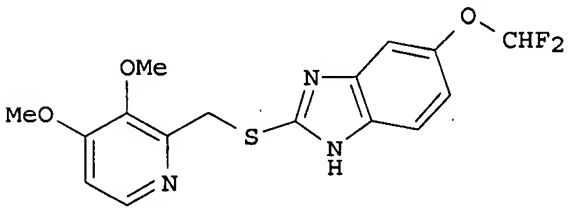
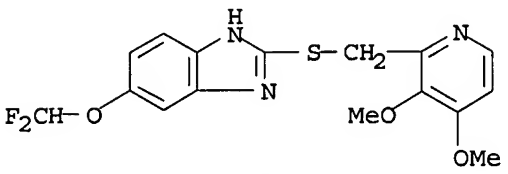


II

AB The invention relates to a novel process for preparing (S)-pantoprazole (I) via stereoselective oxidation of pyridinylmethylsulfinylbenzimidazole derivative
in the presence of L-tartaric acid derivative and chiral zirconium or hafnium catalyst. For instance, the title compound I, useful as proton pump inhibitor, was prepared from thiobenzimidazole derivative II in the presence of L-tartaric acid amide via Zr(IV) isopropoxide catalyzed oxidation

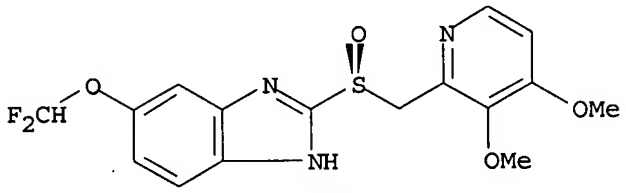
by cumene hydroperoxide with a yield of 80% (optical purity was >98%, example 3).

RX(1) OF 1



(step 1)

1. C:63126-10-3, i-BuCOMe
2. C:23519-77-9, Me2CHOH
3. EtN(Pr-i)2, Cumene hydroperoxide, S:98-82-8
4. NaHCO3, Na2S2O3, Me2CHOH, Water



82%

NOTE: optimization study, optimized on catalyst, stereoselective
CON: STAGE(1) 40 - 45 deg C
STAGE(2) 40 - 45 deg C; 1 hour; 30 deg C
STAGE(3) 20 hours, 30 deg C

=>